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13. ABSTRACT (Maximum 200 words)

Our work on moving interface problems in materials science combines fast PDE solvers such as boundary integral methods with fast geometric algorithms and semi-Lagrangian implicit representations to build effective numerical methods.

We developed an implicit boundary integral method for computing periodic dendrite formation in the symmetric model of unstable solidification [7] and fast algorithms for evaluating heat potentials [2] which speeded up our method by several orders of magnitude. In [6], we combined the boundary integral method of [7] with fast algorithms from [2,3,8] and the level set method of [4]: the level set method handled topological changes effectively while fast boundary integral techniques ensured accuracy and efficiency in the velocity evaluation. We developed and analyzed efficient and accurate new vortex methods for modeling convection in the melt [4,10,11], together with new error analyses [12] and quadrature rules [9] for general integral equations. Since 1999, we have focused on the development and implementation of highly effective new numerical methods for general moving interface problems and widely applicable subsidiary computations. We summarize three projects below: the fast modular semi-Lagrangian method for general moving interfaces (described in Publications [P112] and references [13-16]), accurate contouring methods in two and three dimensions, and fast solution of two-point boundary value problems [P3,P4].

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NUMERICAL METHODS FOR SOLIDIFICATION PROCESSES IN MATERIALS SCIENCE

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Objectives Our overall goal is to develop, implement and transfer accurate new numerical methods for solving moving boundary problems in materials science. We have three specific objectives:

- Combine semi-Lagrangian time stepping, accurate contouring and fast geometric algorithms to develop and implement accurate, efficient and general new methods for moving sharp interfaces.
- Develop a fast modular moving interface code for transfer to other researchers, labs, and industry.
- Build efficient, accurate and general integral solvers for coupled nonlinear systems of Poisson and heat equations modeling common material phenomena, and couple these solvers to our modular moving interface code.

Status of Effort We have attained our first objective—an accurate, efficient and general moving interface method—with the semi-Lagrangian contouring method reported in Publication [P1]. We are developing a portable C code with fast accurate contouring techniques based on deferred correction schemes, and fast PDE solvers based on integral equation techniques, to complete our second and third objectives.

Accomplishments Our work on moving interface problems in materials science combines fast PDE solvers such as boundary integral methods with fast geometric algorithms and semi-Lagrangian implicit representations to build effective new numerical methods.

We developed an implicit boundary integral method for computing periodic dendrite formation in the symmetric model of unstable solidification [7] and fast algorithms for evaluating heat potentials [2] which speeded up our method by several orders of magnitude. In [6], we combined the boundary integral method of [7] with fast algorithms from [2,3,8] and the level set method of [4]: the level set method handled topological changes effectively while fast boundary integral techniques ensured

accuracy and efficiency in the velocity evaluation. We developed and analyzed efficient and accurate new vortex methods for modeling convection in the melt [4,10,11], together with new error analyses [12] and quadrature rules [9] for general integral equations. Since 1999, we have focused on the development and implementation of highly effective new numerical methods for general moving interface problems and widely applicable subsidiary computations. We summarize three projects below: the fast modular semi-Lagrangian method for general moving interfaces (described in Publications [P1,P2] and references [13–16]), accurate contouring methods in two and three dimensions, and fast solution of two-point boundary value problems [P3,P4].

Moving interface problems A moving interface is a collection $\Gamma(t)$ of nonintersecting oriented closed curves (in \mathbf{R}^2) or surfaces (in \mathbf{R}^3). A sufficiently smooth moving interface has an outward unit normal vector N , a mean curvature C , and a normal velocity vector VN . A moving interface problem specifies VN as a functional of $\Gamma(t)$. Examples include passive transport $V = N \cdot F$ where $F(x, t)$ is given, geometric motion $V = p(\theta) - q(\theta)C$ where $\cos \theta = N \cdot \hat{x}$, Ostwald ripening $V = \left[\frac{\partial u}{\partial N} \right]$, where u solves the Laplace equation $\Delta u = 0$ off $\Gamma(t)$ and $u = C$ on $\Gamma(t)$, and models for crystal growth $V = \left[\frac{\partial u}{\partial N} \right]$, where u solves the heat equation $u_t = \Delta u$ off $\Gamma(t)$ with the geometric boundary condition $u = f(N, C, V)$ on $\Gamma(t)$.

The implicit approach Any moving interface problem can be reformulated as a PDE for a function φ whose zero set is $\Gamma(t)$. The normal, curvature and velocity are then

$$N = \frac{\nabla \varphi}{\|\nabla \varphi\|}, \quad C = -\nabla \cdot N, \quad VN = \frac{\varphi_t \nabla \varphi}{\|\nabla \varphi\|^2}.$$

Given an extension of VN off $\Gamma(t)$ to a globally defined function W , we can regard the VN formula as a PDE for φ :

$$\varphi_t - W \cdot \nabla \varphi = 0.$$

We solve this equation on an adaptive quadtree mesh to eliminate the cost of going up a dimension. Correct viscosity solutions are obtained by semi-Lagrangian time stepping with exact distancing and large time steps. A general problem-independent velocity extension makes our method modular and easy to apply.

Semi-Lagrangian methods The semi-Lagrangian ‘‘CIR’’ method [1] solves $\varphi_t - F(x, t) \cdot \nabla \varphi = 0$ by the following algorithm: at each x in the grid, move x back with velocity $F(x, t_n)$ to $s = x + kF(x, t_n)$; interpolate $\varphi(x, t_n)$ to the point s ; set $\varphi(x, t_{n+1})$ equal to the interpolated value. Our second-order time stepping scheme couples a CIR predictor with a trapezoidal corrector using the velocity evaluated from the CIR approximation. It combines the unconditional stability of CIR with the dramatically reduced dissipation of the trapezoidal rule. Interpolation error is eliminated by exact distance finding in a dynamic quadtree data structure.

We first tested the semi-Lagrangian approach in [13] by solving level set equations with a fixed uniform mesh and ENO differencing. Second, we developed an efficient

new redistancing technique with the aid of a new quadtree structure whose cells know the signed distance to nearby elements of $\Gamma(t)$. The quadtree is built in $O(N \log N)$ work by a three-step recursive search procedure. Computations of moderate complexity are speeded up 400 times, while redistancing the CIR method on a uniform mesh costs considerably less than moving φ one step [14]. Third, the semi-Lagrangian method of [15] combined CIR with an adaptive quadtree mesh to build a method which is not only accurate and robust but also optimally efficient: an interface $\Gamma(t)$ with N degrees of freedom costs only $O(N \log N)$ to move one step. Efficiency is further enhanced by the unconditional stability of the semi-Lagrangian time stepping scheme: large time steps $k = O(h)$ can be taken even on refined meshes. The tree mesh is refined with a functional approach: given a signed distance function $\varphi(x, t_n)$, we build a tree at time $t_{n+1} = t_n + k$ by recursive evaluation of $\varphi(x, t_{n+1}) = \varphi(s, t_n)$ at projected points $s = x + kF(x, t_n)$. The criterion for splitting a tree cell is simple: the values of $\varphi(x, t_{n+1})$ on the cell are smaller than the size of the cell.

Our semi-Lagrangian method for moving interfaces [16] combines efficient exact quadtree-based redistancing, stable second-order semi-Lagrangian time stepping, a modular problem-independent velocity extension, and exact φ interpolation in the CIR scheme. The velocity extension technique evaluates the nearest-point extension on a distance tree, builds a continuous interpolant, and satisfies a maximum principle. Our method resolves and moves complex interfaces at optimal cost with time steps unconstrained by numerical stability. It is a “black-box” method for moving interfaces, which accepts the interface and its velocity at time t and returns the evolved interface one time step later. Such methods simplify moving interfaces, because the numerics are independent of the physical problem driving the interfacial motion. Numerical results show that the method converges to correct viscosity solutions even for difficult moving interface problems involving merging, faceting, transport, nonlocality and anisotropic curvature-dependent geometry.

A fast semi-Lagrangian contouring method [P1] General moving interface problems are solved in [P1] by a new approach: extract the moving interface from an explicit semi-Lagrangian advection formula with efficient geometric algorithms and fast accurate contouring techniques. A modular adaptive implementation with fast new geometry modules computes highly accurate solutions to moving interface problems involving merging, anisotropy, faceting, curvature, dynamic topology and nonlocal interactions of PDE type. Exact geometric algorithms are tuned for speed; velocity evaluation and time stepping are efficiently decoupled from interface resolution; fast new contouring techniques dramatically increase overall accuracy. An efficient adaptive framework combines the high resolution of front tracking with the topological robustness of implicit representations. Currently three projects are underway: application to nonlocal problems such as Ostwald ripening, development of accurate general contouring schemes in two and three dimensions, and fast high-order solution of two-point boundary value problems.

Ostwald ripening [P2] We are building fast nonlocal velocity evaluation modules for the standard moving interface problems of materials science. The simplest example is Ostwald ripening, which models the growth of larger solid drops by evaporation from smaller drops with total solid volume conserved. The velocity V is the normal derivative $\left[\frac{\partial u}{\partial N}\right]$ of the function u which is harmonic off $\Gamma(t)$ and equal to the curvature on $\Gamma(t)$. We evaluate this nonlocal velocity by solving the integral equation of classical potential theory and applying the Dirichlet to Neumann operator. The solution u is a double layer potential

$$D\mu(x) = \int_{\Gamma} \frac{\partial K(x, y)}{\partial N(y)} \mu(y) dy$$

of an unknown density μ on $\Gamma = \Gamma(t)$, with $K(x, y) = \frac{1}{2\pi} \log \|x - y\|$ the free-space Green function for the two-dimensional Laplace equation. The density μ solves the integral equation

$$\frac{1}{2}\mu(x) + \int_{\Gamma} \frac{\partial K(x, y)}{\partial N(y)} \mu(y) dy = C(x), \quad x \in \Gamma.$$

Once μ is found, it is convenient to view the harmonic function u as the real part of an analytic function U . The Cauchy-Riemann equations then yield V as the tangential derivative of the imaginary part of U , which is easier to compute than the normal derivative of the real part u . Discretization of this formulation is highly accurate if the interface is represented by equidistant points in arclength. Detailed resolution of the interface requires many points, so fast algorithms such as the fast multipole method play an important role.

Accurate contouring The general problem of finding a smooth geometrically constrained approximate zero set of a function which can be evaluated at arbitrary points occurs frequently in computational science and requires a robust general contouring package. An ideal contouring package would accept function values (and derivatives if available) at arbitrary points and produce a piecewise-smooth approximation to the zero set with corners where necessary. Geometric constraints such as bounds on curvature away from corners are vital in applications such as computer-controlled machining, and pose a major complication for existing public-domain contouring software. We are developing a generally useful package for constrained piecewise-smooth contouring of scattered data in two and three dimensions, based on new methods of scattered data interpolation and a new floating-point stability analysis of the contouring problem.

Deferred correction solvers for boundary value problems [P3,P4] Contouring on a subdomain requires the solution of a two-point boundary value problem for the curve connecting known zeroes on the subdomain boundary. Thus we have developed efficient and accurate new deferred correction techniques for the solution of the two-point boundary value problem

$$\begin{aligned} y' &= C(t)y + f(t), & a < t < b \\ Ay(a) + By(b) &= g \end{aligned}$$

for a vector-valued function $y : [a, b] \rightarrow R^q$. Deferred correction is a strategy of systematically promoting a low-order scheme such as the midpoint rule to an efficient high-order scheme, by applying the same basic scheme to solve an equation for the error in terms of the residual. The error equation is solved efficiently by repeated use of a highly stable block arrowhead QR factorization. This approach yields stable, efficient and highly accurate schemes of orders up to 20, with naturally adapted grids. Fig. 1 illustrates the speed and accuracy of these schemes, applied to difficult and singular problems which challenge standard packages [P3]. A new convergence theory confirms these experimental results [P4].

The future Planned future developments include higher-order accurate contouring and boundary representations with constrained geometry, three-dimensional implementation, and applications to PDE-type problems where the moving interface is coupled to complex materials science.

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Interactions/Transitions The PI presented results from this research in seminars and colloquia at Argonne National Laboratory, Lawrence Berkeley National Laboratory, Brown University, California Institute of Technology, the University of Arizona, UC Berkeley, the University of Chicago, and the University of Oregon.

Publications [P1] J. Strain. A fast semi-Lagrangian contouring method for moving interfaces. *J. Comput. Phys.*, 169:321–342, 2001.

[P2] J. Strain. Fast solution of nonlocal moving interface problems. To be submitted to *J. Comput. Phys.*, July 2002.

[P3] J. Strain. Fast stable deferred correction methods for two-point boundary value problems. To be submitted to *ACM Trans. Math. Softw.*, May 2002.

[P4] A. C. Hansen and J. Strain. Convergence of deferred correction methods. To be submitted to *BIT*, August 2002.

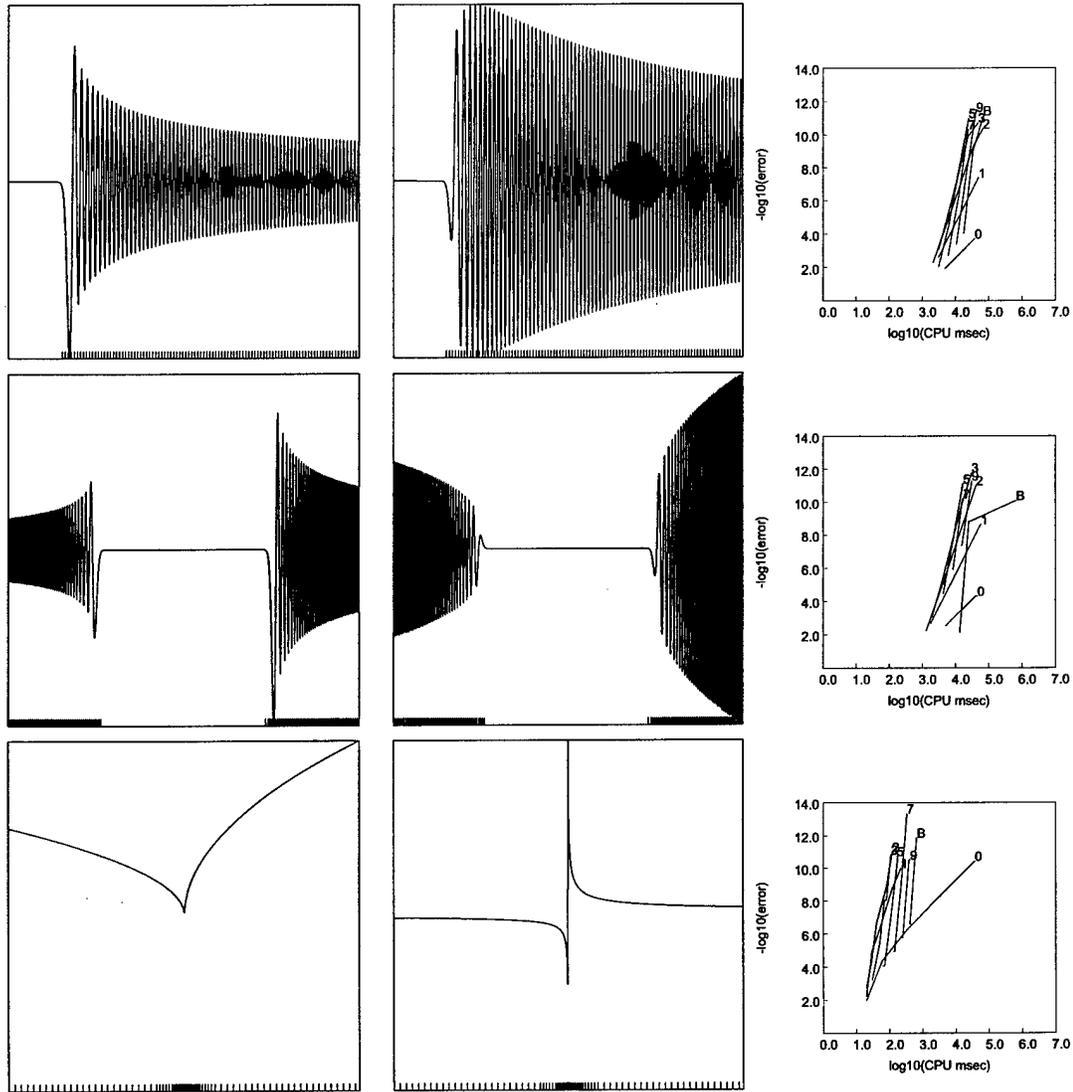


Figure 1: Grid with solution, derivative, and correct digits vs. logarithm of CPU time for adaptive deferred correction schemes of orders 2 through 20, applied to Bessel functions, Airy functions, and parabolic cylinder functions with a singular cusp.